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This final report contains a permanent record of the progress and significant accomplishments in performance of the research effort. The primary focus of this research project has been the design and testing of new algorithms for matrix computations with particular applications to least squares and optimization methods in structural analysis, Markov analysis, signal processing and related problems in science and engineering. The objectives were to develop, test, and analyze fast numerical algorithms for the efficient solution to large scale problems on modern high performance architectures. (JES)

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Fast Algorithms for Structural Optimization, Least Squares and Related Computations

Robert J. Plemmons

September 1988

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Table of Contents

1. Summary of Major Accomplishments

The primary focus of this research project has been the design and testing of new algorithms for matrix computations with particular applications to least squares and optimization methods in structural analysis, Markov analysis, signal processing and related problems in science and engineering. The objectives were to develop, test, and analyze fast numerical algorithms for the efficient solution to large scale problems on modern high performance architectures.

Researchers in scientific computation recognize that to achieve the speeds necessary to solve the new complex scientific and engineering problems of significant impact, requires radical reorganization of traditional algorithms in matrix analysis. New fast algorithms for the modern generation of supercomputers (such as the Cray X-MP) and mini-supercomputer systems (such as the Alliant FX/8) as well as distributed memory multiprocessor systems (such as the iPSC Hypercube), are essential. In order to meet the challenges of this emerging new generation of machines, it has been the goal of this project to develop techniques in matrix computations for efficient implementation on advanced architectures. Significantly, applications of our work to the practical real-world problems of structural optimization and least squares estimation methods in signal processing have been made. In the area of structural analysis we are concerned with the fundamental problem of elastic analysis - that of finding the stresses and strains and solving optimal redesign problems, given a finite element model of a large complex structure and a set of external loads. To obtain the solution of this constrained minimization problem, a variety of algorithms involving the displacement method or the force method can be applied. While the advantages of implementing one of these methods over the other on serial computers have been widely studied, the effects of parallelism in performing the matrix computations have not received a great deal of attention until recently. Our work on this topic has led to publications in journals such as **Computer Methods in Applied Mechanics and Engineering**, the **International Journal on Numerical Methods in Engineering**, **Numerische Mathematik**, the **SIAM Journal on Algebraic and Discrete Methods**, and the **SIAM Journal on Scientific and Statistical Computing**. Our main objective in least squares computations has been to develop fast recursive orthogonal and hyperbolic rotation algorithms for signal processing. Our schemes are amenable to implementation on a variety of vector and parallel processing systems, such as the Alliant FX/8 and the Intel iPSC Hypercube. This work in developing near real-time algorithms has produced some especially important

recent results which have or will appear in such journals as **Computational and Applied Mathematics, ICASSP 87: Proc. IEEE Conf. on Acoustics, Speech and Signal Processing, Linear Algebra and Its Applications Special Issue on Electrical Engineering,** and the **SIAM J. on Scientific and Statistical Computing.** A total of 32 publications involving the principal investigator have resulted from this 5-year AFOSR sponsored project which began in the middle of 1983.

Some highlights of this research are given next. The referenced publications can be found in Section 8.

- **Force Method Computations in Structural Mechanics:**

Historically there are two principal methods of matrix structural analysis, the displacement (or stiffness) method and the force (or flexibility) method. In joint work with M. T. Heath and R. C. Ward at the ORNL, we have given some implementations of the force method which are numerically stable and preserve sparsity. These factors have led to serious deficiencies in the force method in the past. The approach here was to carry out the computations using orthogonal factorization techniques recently developed for least squares computations. Other work on the force method has involved the development and testing of algorithms to compute a sparse basis of the null space. More general applications of this work also exist in quadratic programming. Implementations of the, so-called, turnback algorithm for banded equilibrium matrices **E** arising in finite element problems were made on a variety of systems, including a Denelcor HEP multiprocessor and an Alliant FX/8 by the graduate student M. W. Berry. (See publication nos. 1, 4, 7, 9, 10 and 11 listed later.)

- **Computational Structural Mechanics on High Performance Architectures:** The major focus of this work is a detailed study of the vectorization and parallelization of new and existing variations of the Displacement and Force Methods in the engineering analysis of large-scale structures. Considering the increasing demands on the structural engineer to analyze larger and more complex structures, the need for vectorization and/or multiprocessing of the numerical schemes is essential. We have used two high performance architectures in this work: an Alliant FX/8 and a Cray X-MP (made available by the NSF at the University of Illinois NCSA). Implementation and performance evaluations for a variety of approaches on these architectures have indicated that an element-by-element preconditioned conjugate gradient scheme produces superior performance. Some of the results of this study were presented at the First World Congress on Computational Mechanics at Austin ,TX. This work includes a joint project with M. W. Berry at the Illinois CSRD. (See publications 13, 18 and 20.)

• **Direct-Iterative Methods for Large-Scale Least Squares Problems:** In 1975 Chen and Gentleman suggested a 3-cyclic SOR method for solving least squares problems, based on a partitioning scheme for the observation matrix A into the column 2-block form $A = [A_1\ A_2]^T$ where A_1 is square and nonsingular. This combined direct-iterative method was discussed further and applied to angle adjustment problems in Geodesy by Plemmons in 1979. Later, Niethammer, de Pillis and Varga corrected a mistake in that study and extended the SOR convergence interval. In the present joint work with T. L. Markham and M. Neumann, a 2-cyclic SOR method is suggested and shown to have a superior asymptotic convergence rate over the 3-cyclic scheme. (See publication 8.)

• **Iterative Methods for Equality Constrained Least Squares Problems:** We consider the equality constrained least squares problem (LSE) of minimizing the norm $\|c - Gx\|_2$ subject to the constraint $Ex = p$. A preconditioned conjugate gradient method is applied to the Kuhn-Tucker equations associated with the LSE problem. This method is compared to a block SOR method and is clearly superior to it. We show that the method is well suited for structural optimization problems in reliability analysis and optimal design. Numerical tests on an Alliant FX/8 and a Cray X-MP using some practical structural analysis data exhibit the efficiency of the method. Applications also have been made to filtering methods in signal processing. Here the scheme has the definite advantage that the solution x is easy to update after a rank one modification of the matrix G . This is joint work with J. Barlow at Penn State University and Nancy Nichols at NCSU. (See publication no. 25.)

• **Least Squares in Geodetic and Related Applications:** This work is concerned with the solution of large-scale least squares problems. Special attention is placed on those least squares problems arising in a variety of scientific and engineering problems, including geodetic adjustments and surveys, medical image analysis, molecular structures, partial differential equations and substructuring techniques in structural engineering. In each of these problems, matrices A often arise which possess a block angular structure which reflects the local connection nature of the underlying problem. In this work, parallel schemes have been suggested for the orthogonal factorization of matrices in block angular form and for the associated backsubstitution phase of the least squares computations. In addition, a parallel scheme for the calculation of certain elements of the covariance matrix is described. It is shown that these algorithms are ideally suited for multiprocessors with three levels of parallelism

such as the Cedar system. This is joint work with A. Sameh and G. H. Golub. (See publication nos. 15 and 17.)

- **Computing Stationary Distributions of Markov Chains:**

In a series of papers we have investigated both direct and iterative methods for computing the limiting probabilities (stationary distributions) of finite Markov chains. Such computations are important in the analysis of many models in the mathematical sciences, such as queueing network models, input-output economic models and compartmental tracer analysis models. Topics considered include: (1) convergent iterations for large-scale queueing problems, (2) a combined direct-iterative method for certain M-matrix linear systems, and (3) updating LU factorizations for computing stationary distributions (joint with R. E. Funderlic). (See publication nos. 2, 3, 5, 6, 12 and 14.)

- **A Two-Level Preconditioned Conjugate Gradient Scheme:**

The conjugate gradient algorithm is one of the most efficient methods for solving a variety of problems arising in signals, systems and control, and it has been successfully implemented on various vector computers. In part as an effort to efficiently implement this algorithm on parallel processors, a two-level preconditioning scheme is proposed here and tested on an Alliant FX/8 multiprocessor system. The scheme is based on applying the SSOR and incomplete Cholesky preconditioners simultaneously to a partitioned form of the coefficient matrix A. The two-level preconditioner appears to be especially well-suited for the case where A has a bordered block diagonal form commonly arising in domain decomposition or substructuring type problems. This is joint work with the former Ph.D. student D. J. Pierce who is now with Boeing Computer Services. (See publication 22.)

- **Parallel Multisplitting Iterative Methods:**

Despite the major recent activity in parallel processing, few effective new algorithms designed exclusively for multiprocessors have been put forth. One such is the multisplitting iterative scheme suggested originally by D. O'Leary and R. White. Here the coefficient matrix A is split into several carefully chosen splitting forms $A = M_i - N_i$, $i = 1,\dots,p$, and iterations are performed on separate processors. In this joint work with M. Neumann, convergence of such schemes is studied in detail for the case where A is an M-matrix. It is shown how load balancing can be achieved without reducing the overall convergence rates. (See publications 16 and 19.)

• **Analysis of a Hyperbolic Rotation Algorithm for Signal Processing:** The application of hyperbolic plane rotations to the least squares downdating problem arising in windowed recursive signal processing is studied. A forward error analysis is given to show that the algorithm can be expected to perform well in the presence of rounding errors, provided the problem is not too ill-conditioned. The hyperbolic rotation algorithm is shown to be forward (weakly) stable and, in fact, comparable to an orthogonal downdating method shown to be backward stable by Stewart. Numerical comparisons are made with Stewart's method as implemented in LINPACK. These tests collaborate our error analysis which indicates that the two methods should result in similar accuracy. However, the hyperbolic scheme under consideration requires $\frac{n^2}{2}$ fewer multiplications for each downdating step, where n is the number of least squares filter coefficients. In addition, it is much more amenable to implementation on a variety of vector and parallel machines. This is joint work with the former Ph.D. student C.-T. Pan and with S. T. Alexander from the NCSU Department of Electrical and Computer Engineering. (See publications 21 and 23.)

• **Parallel Factorization Schemes for Minimizing Sums of Euclidean Norms:** The problem of minimizing a weighted sum of Euclidean norms is considered. Applications include minimal surface computations. A robust parallel algorithm, based on the line-search Newton's Method, has been developed which takes advantage of the structure of the problem in order to fully utilize vectorization and concurrency in the computations. The method can achieve high performance, especially on a machine with an architecture that combines vector and parallel capabilities on a two-level shared memory structure, such as that present on the Alliant FX/8 system where our tests were made. This is joint work with S. J. Wright at NCSU. (See publication 24.)

• **Rank One Matrix Modifications on Dist. Memory Architectectures:** Here we are developing and testing parallel least squares updating and downdating schemes on a 64 node Intel Hypercube. The purpose is to design near real-time algorithms for signal processing applications. The results thus far have been very encouraging. One of the students who is involved with this project spent the Summer of 1987 at Oak Ridge developing code on their iPSC64 system. This is joint work with the student C. Henkel, who is majoring in Nuclear Engineering at NCSU, and M. T. Heath at the Oak Ridge National Laboratory. The paper was given as an invited lecture at the Hypercube 3 Conference, Cal. Tech., Jan. 1988. (See publication 26.)

• **Parallel Least Squares Modifications Using Inverse Factorizations:** The process of modifying least squares computations by updating the covariance matrix has been used in control and signal processing for some time in the context of linear sequential filtering. Here we give an alternative derivation of the process and provide extensions to downdating. Our purpose is to develop algorithms that are amenable to implementation on modern multiprocessor architectures. In particular, the inverse Cholesky factor $\mathbf{R}^{-1}$ is considered and it is shown that $\mathbf{R}^{-1}$ can be updated (downdated) by applying the same sequence of orthogonal (hyperbolic) plane rotations that are used to update (downdate) $\mathbf{R}$. We have attempted to provide some new insights into least squares modification processes and to suggest parallel algorithms for implementing Kalman type sequential filters in the analysis and solution of estimation problems in control and signal processing. This is joint work with former Ph.D. student C.-T. Pan. (See publication 27 .)

• **Optimality Relationships for p-Cyclic SOR:** The optimality question for block p-cyclic SOR iterations discussed by Young and by Varga is answered under general conditions on the spectrum of the block Jacobi matrix. In particular, it is shown that repartitioning a block p-cyclic matrix into a q-cyclic form, $q < p$, always results in asymptotically faster SOR convergence for the same amount of work per iteration. As a consequence **block 2-cyclic SOR is optimal.** This is joint work with D. Pierce. (See publication 29.)

• **Recursive Least Squares Filtering on a Hypercube Multiprocessor:** We have developed an efficient parallel implementation of an algorithm for recursive least squares computations based upon the covariance updating method. The target architecture system is a distributed memory multiprocessor. Test results on a 64 node iPSC/2 hypercube display the parallel efficiency of the algorithm. This **64 node system** is measured to execute the algorithm over 48 times as fast as a single processor when the problem size for the system is fixed (fixed size speedup) and over **61 times as fast as a single processor** when the problem size per processor is fixed (scaled speedup). Applications include robust regression in statistics and modification of the Hessian matrix in optimization, but the primary motivation for this work is the need for near real-time recursive least squares computations in signal processing. This work is **strong evidence of the power of distributed memory computing in recursive least squares filtering** applications. (See publications 28 and 30.)

• **Parallel Computation of the Nullspace for Equilibrium Matrices:** Equations of equilibrium arise in numerous areas of engineering. Applications to electrical networks, structures and fluid flow are elegantly described in a recent book on applied mathematics by Strang. The context in which equilibrium equations arise may be stated in two forms:

Constrained Minimization Problem: $\min (x^T A x - x^T r)$ subject to $Ex = s$,
Lagrange Multiplier Problem: $EA^{-1}E^T\lambda = s - EA^{-1}r \quad Ax = r - E^T\lambda$.

Here A is generally some symmetric positive definite matrix associated with the minimization problem. For example, A is the element flexibility matrix in the structures application. An important approach to the solution to such problems involves dimension reduction nullspace schemes based upon computation of a basis for the nullspace for E. An equilibrium matrix (or incidence matrix) may be assumed to have entries plus or minus 1 and be of full row rank. In our approach to solving such problems we emphasize the **parallel computation** of a basis for the nullspace of E and examine the applications to structural optimization and fluid flow. Several new block decomposition and node ordering schemes are suggested. Comparisons of our schemes are made with those of Pothen, et al, for structures and Hall, et al, for fluids. This is joint work with R. E. White. (See publication 31.)

2. Faculty Associate

- Robert E. White, Summer 1988.

3. Graduate Students

- Michael. W. Berry, M.Sc. 1985. Now at the University of Illinois Center for Supercomputing Research and Development, Urbana, IL.
- Daniel. J. Pierce, Ph.D. 1986. Now at the Boeing Comp. Serv., Seattle, WA.
- C.-T. Pan, Ph.D. 1987. Now at Northern Illinois University, DeKalb, IL.
- William R. Ferng, Ph.D. (expected) 1989. Graduate Research Assistant.
- Douglas James, Ph.D. (expected) 1990. Major, US Air Force. Graduate Air Force Fellowship Awardee.

4. Conference Lectures

- AFOSR Conference on the Impact of Large-Scale Computing on Air Force Research and Development, Kirtland AFB, Albuquerque, NM February(1984).
- NSF Workshop on Very Large Least Squares Problems and Supercomputing, Purdue University, Lafayette, IN March(1984).
- Gatlinburg IX, Warerloo, Ontario, Canada July(1984).
- AMS/SIAM Conference on Linear Algebra in Systems Theory, Bowdoin, ME August(1984).
- SIAM Conference on Algorithms and Architectures for Parallel Processing - Minisymposium on Parallel Linear Algebra, Norfolk, VA November(1985).
- NSF Conference on Matrix Theory, Auburn, AL March(1986).
- Workshop on Industrial Applications of Signal Processing, Raleigh, NC April(1986).
- Workshop on Scientific Applications and Algorithm Design for High Speed Computation, Urbana, IL April (1986).
- SIAM Conference on Linear Algebra in Signals, Systems and Control - Special Session on Signals, Boston, MA August(1986).
- First World Congress on Computational Mechanics, Austin , TX, September (1986).
- ICIAM'87 Minisymposium on Linear Algebra in Systems and Control, Paris, June (1987).
- Inter. Conf. on Lin. Alg. in Systems and Control, Valencia, Spain, September(1987).

- Gatlinburg X, Fairfield Glade, TN, October (1987).
- Conference on Numerical Linear Algebra and Parallel Computation, Oberwolfach, Germany, March(1988).
- Seminar on Iterative Methods for Singular Systems, Karlsruhe, Germany, March(1988).
- Cray Workshop on Supercomputer Applications of Sparse Matrix Algorithms, Santa Cruz, CA, April(1988).
- Southeastern AMS Meeting - Special Session on Numerical Linear Algebra, Knoxville, TN, April(1988).
- DOE Workshop on Least Squares Computations (5 lectures), Knoxville, TN, May(1988).
- International Conference on Computational and Applied Mathematics, Belgum July(1988) .
- NATO Workshop on Numerical Linear Algebra, Signal Processing and Parallel Algorithms, Belgium July(1988).

5. Colloquium Lectures

- University of Wisconsin-Madison 1984.
- Pennsylvania State University 1984.
- Ohio University 1984.
- University of Illinois-Urbana 1985.
- University of Virginia 1985.
- Wake Forest University 1986.
- Argonne National Laboratory, Argonne, IL (1986).
- Air Force Office of Scientific Research, Bolling Air Force Base, DC (1987).
- INRIA, Rennes University, Rennes, France (1987).
- Valencia Polytechnic Institute, Valencia, Spain, September (1987).
- University of Illinois-Urbana 1988.

6. Consulting and Advisory Functions at DOD Installations

- Kirtland Air Force Base, Albuquerque, NM, February (1984).
- Wright-Patterson Aeronautical Laboratories, Wright-Patterson, OH, January(1988).
- NATO Scientific Affairs Division, Brussels, Belgium, July(1988).

7. Related Professional Activities

- Editorial Board, SIAM J. on Algebraic and Discrete Methods.
- Associate Managing Editor, SIAM J. on Matrix Analysis and Applications.
- Advisory Editor, Linear Algebra and Applications.
- Chairman, SIAM Activity Group on Linear Algebra 1983-86.
- Conference Organizing Committees:
  - SIAM Conference on Applied Linear Algebra, Madison, WI 1988.
  - International Conf. on Finite Element Methods in Flow Problems, Huntsville, AL, 1988.
  - ICIAM'87, Minisymp. on Linear Algebra in Systems and Control, Paris 1987.
  - First World Congress on Computational Mechanics - Special session on Parallel Algorithms, Austin, TX, 1986.
  - SIAM Conference on Linear Algebra in Signals, Systems and Control, Boston, MA,1986.
  - SIAM Conference on Applied Linear Algebra, Raleigh, NC, 1985.
  - AMS Conference on Linear Algebra in Signals, Systems and Control, Bowdoin, MI, 1984.
- Elected Member, SIAM Council, 1985 - 87, 1988 - 90.
- Elected Member, SIAM Board of Trustees, 1988 - 90.

8. Publications on Research Supported by Grant

1. *Sparse orthogonal schemes for structural optimization using the Force Method*, **SIAM J. Sci. and Stat. Comp.**, 5(1984), 514-532 (with M. T. Heath and R. C. Ward).

2. *A combined direct-iterative method for certain M-matrix linear systems*, **SIAM J. Alg. and Disc. Meth.**, 5(1984), 33-42 (with R. Funderlic).

3. *Comparison of some direct methods for computing stationary distributions of Markov chains*, **SIAM J. Sci. and Stat. Comp.**, 5(1984), 453-469 (with W. Harrod).

4. *Comparison of some orthogonal schemes for structural optimization*, **Proc. Army Conf. on Applied Mathematics and Computing - Washington DC**, (1984), 477-485 (with M. W. Berry, M. T. Heath and R. C. Ward).

5. *Convergence of Gauss-Seidel iterations for computing stationary distributions of Markov chains*, **Proc. Inter. Conf. on Linear Algebra and Applications - Vitoria Spain**, (1984), 101-116 (with G. P. Barker).

6. *Backward error analysis for linear systems associated with inverses of M-matrices*, **BIT**, 24(1984), 102-112 (with M. Neumann).

7. *Minimum norm solutions to linear elastic analysis problems*, **Inter. J. Numer. Meth. in Engineering**, 20(1984) 983-998 (with I. Kaneko).

8. *Convergence of direct-iterative methods for large-scale least squares problems*, **Lin. Alg. and Applic.**, 69(1985), 155-167 (with T. Markham and M. Neumann).

9. *An algorithm to compute a sparse basis of the null-space*, **Numerische Mathematik**, 47(1985), 483-503 (with M. Berry, I. Kaneko, M. Heath, M. Lawo and R. Ward).

10. *Parallel schemes for finite element structural analysis on the HEP multiprocessor*, **Proc. Workshop on the Denelcor HEP**, Norman, OK (1985), 157-180 (with M. Berry).

11. *Computing a banded basis of the null space*, **Proc. AMS/SIAM Conf . on the Role of Linear Algebra in Systems Theory - Bowdoin ME, Contempory Mathematics**, 47(1985), 7-25 (with M. W. Berry).

12. *Updating methods for computing stationary distributions*, **SIAM J. Alg. and Disc. Meth.**, 7(1986), 30-42 (with R. Funderlic).

13. *A parallel block iterative method applied to computations in structural analysis*, **SIAM J. Alg. and Disc. Meth.**, 7(1986), 337-347.

14. *Convergent iterations for computing stationary distributions*, **SIAM J. Alg. and Disc. Meth.**, 7(1986), 390-398 (with G. Barker).

15. *Least squares computations for Geodetic and related problems*, **Proc. Workshop on Sci. Applic. and Alg. Design for High Speed Computing**, Urbana , IL (1986).

16. *Convergence of parallel multisplitting iterative methods*, **Lin. Alg. and Applic**, 88(1987), 39-49 (with M. Neumann).

17. *Parallel block schemes for large-scale least squares computations*, **Proc. Workshop on Sci. Applications and Alg. Design for High speed Computing - Urbana IL**, (1987) (with G. H. Golub and A. Sameh).

18. *A conjugate gradient method for equality constrained least squares*, **Proc. Conf. on Advanced Algorithms and Architectures for Signal Processing - San Diego CA**, 696(1986), 23-30 (with J. Barlow and N. Nichols).

19. *Parallel multisplitting iterative methods*, **Proc. Conf. on Matrix Theory - Auburn AL, Current Trends in Matrix Theory**, Ed. F. Ulig and R. Grone, 1987, 251-254.

20. *Algorithms and experiments for structural mechanics on high performance architectures*, **Comp. Meth. in Appl. Mech. and Eng.**, 64(1987), 487-507 (with M. W. Berry).

21. *Numerical properties of a hyperbolic rotation scheme for windowed RLS filtering*, **Proc. IEEE Conf. on Acoustics, Speech and Signal Processing - Dallas TX**, 1(1987), 423-426 (with S. T. Alexander and C.-T. Pan).

22. *A two-level preconditioner for conjugate gradients*, **Proc. Conf. on Linear Algebra in Signals, Systems and Control, SIAM Press**, 1988, 170-185 (with D.Pierce).

23. *Analysis of a recursive least squares hyperbolic rotation algorithm for signal processing*, **Lin. Alg. and Applic. Special Issue on Electrical Engineering**, 98(1988), 3-40 (with S. T. Alexander and C.-T. Pan).

24. *An efficient parallel scheme for minimizing a sum of Euclidean norms*, **Lin. Alg. and Applic.**, to appear 1988 (with S. J. Wright).

25. *Conjugate gradient methods for equality constrained least squares*, **SIAM J. on Sci. and Stat. Comp.**, to appear 1988 (with J. Barlow and N. Nichols)

26. *Parallel least squares modifications using inverse factorizations*, **Comp. and Appl. Math.**, to appear 1988 (with C. Pan).

27. *Cholesky downdating on a Hypercube*, **ACM Proc. Hypercube 3 Conf.**, Cal. Tech. 1988 (with C. Henkel and M. T. Heath).

28. *Recursive least squares computations on distributed memory multiprocessors*, submitted to **Inter. J. Parallel Processing** (with D. Agrawal and S. Kim).

29. *Optimality criteria for p-cyclic SOR*, submitted to **Numer. Math.** (with D.J. Pierce).

30. *Recursive least squares on a hypercube multiprocessor using the covariance factorization*, submitted to **SIAM J. on Sci. and Stat. Comp.** (with C. Henkel).

31. *Parallel Computation of the Nullspace for Equilibrium Matrices*, to be submitted (with R. E. White).

32. *Parallel algorithms for numerical linear algebra*, in prepatation for the **SIAM Review** (with K. Gallivan and A. Sameh).